USING AN ORGANIC SCAFFOLD TO MODULATE THE QUANTUM STRUCTURE OF AN INTRAMOLECULAR PROTON BOND: CRYOGENIC VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF H_2 ON PROTONATED 8-NAPHTHALENE-1-AMINE

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The quantum structure of the intermolecular proton bond is a key aspect in understanding proton transfer events that govern the efficiency of fuel cells and various biological membranes. Previously, we have constructed a soft binding motif, that consists of a point contact between the lone pairs of two small molecules (combinations of ethers, alcohols, ammonia, and water) that are linked by a shared proton [*Science* 2007, *613*, 249]. Although the frequency of the shared proton vibration has been correlated with effects of acid and base structure, such as proton affinities and dipole moments, the spatial arrangement of the proton donor and acceptor remains unexplored. Towards this aim, we have obtained a molecule of rigid topology that contains a proton donor and acceptor capable of intramolecular proton-bonding (protonated 8-flouronaphthalene-1-amine). Using electrospray ionization coupled with a novel cryogenic mass spectrometry scheme, we employ vibrational predissociation spectroscopy of H_2 tagged ions to elucidate how a forced spatial configuration of the acid and base perturbs the energetics of the proton bond.